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Insights into Inverse Materials Design from Phase Transitions in Shape Space[1] ROSE CERSONSKY, GREG VAN ANDERS, PAUL M. DODD, SHARON C. GLOTZER, Univ of Michigan - Ann Arbor — In designing new materials for synthesis, the inverse materials design approach posits that, given a structure, we can predict a building block optimized for self- assembly. How does that building block change as pressure is varied to maintain the same crystal structure? We address this question for entropically stabilized colloidal crystals by working in a generalized statistical thermodynamic ensemble where an alchemical potential variable is fixed and its conjugate variable, particle shape, is allowed to fluctuate. We show that there are multiple regions of shape behavior and phase transitions in shape space between these regions. Furthermore, while past literature has looked towards packing arguments for proposing shape-filling candidate building blocks for structure formation, we show that even at very high pressures, a structure will attain lowest free energy by modifying these space-filling shapes.

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